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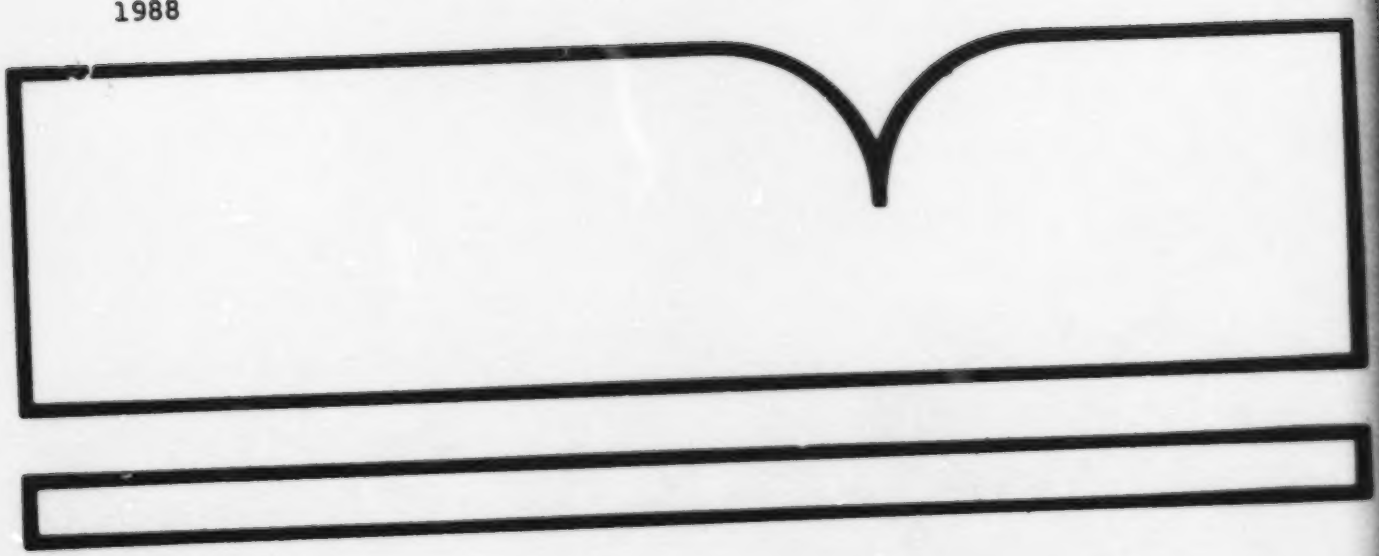

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16. ABSTRACT

This paper is a formal response to the 1988 APCA Critical Review of Ozone Air Quality Models by Dr. John Seinfeld. His Critical Review was a comprehensive discussion on the state of knowledge of urban ozone air quality models. This paper extends Seinfeld's review in the areas of model components and input data, emissions inventories, uncertainties in wind fields, regional scale ozone models, model evaluation, and future research directions.

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OZONE AIR QUALITY MODELS

Critical Review Discussion Papers

The APCA Critical Review entitled "Ozone Air Quality Models" was presented by John H. Seinfeld, Louis E. Nohl Professor and Executive Officer for Chemical Engineering at the California Institute of Technology, Pasadena, California. Dr. Seinfeld presented his review at the 81st APCA Annual Meeting & Exhibition, held in Dallas, Texas in June 1988. The Critical Review paper, published in the May 1988 issue of *JAPCA*, highlighted recent advances and continuing problem areas in photochemical air quality modeling. Prepared discussions and floor comments presented during the Critical Review session in Dallas are published here, along with additional comments and closing remarks by Dr. Seinfeld. Howard M. Ellis, Chairman of the Critical Review Subcommittee of the Publications Committee, served as moderator of the 1988 APCA Critical Review session.

Prepared Discussion

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It is an honor to have been invited to formally discuss Dr. John Seinfeld's Critical Review of Ozone Air Quality Models. Dr. Seinfeld has done an excellent job with a very difficult task. It is difficult in the sense that the development, application, and evaluation of these models demands an interdisciplinary effort involving chemistry, meteorology, engineering, mathematics, statistics, computational methods, systems design, and public policy. A team approach is invariably required in the use of photochemical air quality models, and Dr. Seinfeld has provided us an introduction to the whole team through his comprehensive review. I would like to use this opportunity to expand on a few of the points made in the Critical Review, to add some discussion of regional scale models from my own perspective, and to provide some additional areas where future research is needed.

Model Components and Input Data

Ozone air quality models, or more generally, photochemical air quality simulation models (PAQSMs), are essentially "built" from individual components responsible for simulating specific processes. The process of operator splitting[1] of the governing differential equations in the air quality system to be simulated allows us to consider one process or a subset of processes in any one model component. Dr. Seinfeld gave an overview of the most significant components including transport, chemical production and removal, turbulent dispersion, and deposition. The computational links between components and the numerical methods chosen to solve the principal finite-difference equations are the glue holding the components together.

For some categories of model input data there is a gray area in which the data are sufficiently "processed" before being assimilated by the air quality model itself that the information content of the data is now a combination of measurement/estimation methods and model component processes. Here I am including the data preprocessor(s) upstream of the simulation model itself to be part of the total modeling system. Usually PAQSMs are implemented as a complete system; thus the associated data preprocessors may be thought of as detached components of the PAQSM. Where the data end and the model component assumptions begin is not always clear.

For example, source emissions of ozone precursors are usually provided for major point sources and county-level or gridded area sources. Some models will estimate the plume rise from major point sources and inject these emissions in levels above the surface, while others will lump all emissions together in a relatively deep volume. Some will treat individual point sources with a plume representation at the subgrid scale level (these are hybrid models according to Dr. Seinfeld), while others make no such distinction. The base emissions data are the same in all cases, but models assimilate the data differently. As another example, most PAQSMs need a gridded wind field to drive the transport component. The same set of wind observations may be interpolated and interpreted in different ways by different modeling systems to provide flow fields giving significantly different trajectory paths. These differences are often ascribed to "problems in the data" when, in reality, the assumptions made in the data preparation process are key to understanding the differences. Distinctions such as these between input data and model components must be considered when performing diagnostic analyses on model results.

Chemical kinetic mechanisms are components of all PAQSMs. As stated in the Review, the currently accepted kinetic mechanisms model the ozone profiles from smog

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chamber experiments within about 30 percent for maximum concentrations. This is reasonably good agreement considering that there is a large body of chamber data for ozone extending over a wide range of VOC/NO_x ratios. The intermechanism comparisons for species other than ozone are, however, not as encouraging. Results for species such as PAN, HNO_3, OH, and H_2O_2 vary considerably from mechanism to mechanism for the same set of initial conditions.[2] Insufficient experimental data exist for determining the correct profile of these species. We are left then with a basic modeling question: are we getting the right answer for the right reasons? Until we can verify the chemical mechanisms over a broader range of photochemical species, we cannot answer this question with certainty.

While the development of chemical mechanisms has advanced considerably over the last 15 years, there are still areas that need improvement. A few of these were mentioned in the Review, including a better understanding of the aromatics pathways, the reactions of the larger alkanes, and the photolysis and reactions of the carbonyls. In addition, the chemistry of the natural hydrocarbons should be better represented in the mechanisms. While this may not be a very significant factor for urban scale modeling, initial indications show the natural hydrocarbons to play a large role over regional and continental scales. Explicit mechanisms for isoprene have been postulated,[3] although there are none for the monoterpenes.

Many reaction rate coefficient expressions are not well established, and some contain temperature and pressure dependencies that add considerable uncertainty to their evaluation. For example, the reactions that produce and destroy PAN are strongly temperature sensitive, and the timing and magnitude of the ozone profile is very sensitive to the chemical pathway of PAN. Recently a new temperature-dependent expression was introduced[4] for the PAN production reaction based on empirical evidence from smog chamber work. The new expression shows a stronger temperature effect than the older expression based on kinetic theory, and predicted ozone profiles respond differently depending upon which expression is used. There is, at present, not enough evidence to determine which is the "correct" expression. Further advances in the mechanistic representation of atmospheric chemistry will come with continued basic research including better chamber characterizations and continued experimentation, as well as basic theoretical advances.

I wish to make one final point concerning chemical mechanisms in PAQSMs. Dr. Seinfeld suggests that it is essential that an air quality model accept, as input, text files of the reactions and kinetic parameters in a relatively flexible format. He also says that the program should automatically produce the code to process steady-state species without manual intervention. I agree with these points, although we are still short of reaching this goal. Except for non-grid models, such as EKMA/OZIPP which can afford the luxury of very accurate and flexible yet computationally demanding numerical solvers for chemistry, most PAQSMs employ less rigorous solution methods with algebraic steady-state expressions for the faster-reacting species. The techniques for implementing these methods often depend on the particular mechanism being used, and must be re-evaluated if the mechanism is replaced. Many modelers describe their chemical mechanisms as "modular", implying that it is relatively easy to change from one chemical mechanism to another in a PAQSM. There is still a long way to go before we have truly modular chemical mechanisms. The issues of mechanism integration and solution, initial and boundary condition speciation, and emissions inventory speciation must be adequately addressed before we can easily change kinetic mechanisms in a PAQSM.

Meteorological components of models are also crucial for reasonable ozone predictions. The spatial patterns of predicted concentrations within a model domain are largely governed by the wind field specification. I will elaborate on wind fields later in the discussion of regional models. The representation of the vertical structure of the lower troposphere is a significant aspect of a PAQSM. As Dr. Seinfeld points out, most PAQSMs require a mixing height value at least every hour of the simulation, and preferably spatially resolved over the grid. There are typically few data from which to determine mixing heights at the required resolution; thus the behavior of this parameter can be quite uncertain. The error can be as large as 50 percent during the time when peak ozone concentrations are generated according to Dr. Seinfeld, leading to potentially profound effects on model predictions. The combination of the mixing height at model initialization time and the initial precursor concentrations largely determines the amount of mass within the domain when simulation starts. Since model predictions are often quite sensitive to the initial mass, especially for 24–48 hour simulations, the mixing height must be chosen carefully. Also, outside of the daytime hours of rapid convective and mechanical turnover in the boundary layer, the concept of a well-mixed layer breaks down. Since most models assume good mixing at all times through the layer(s) nearest the ground, we introduce some errors in the physical representation of the mixing process during the early-morning and evening hours. Mixing heights must be analyzed very carefully with as much supporting data as are available when preparing model inputs. In future years, with the increased availability of remote sensing of the boundary layer, perhaps on a regular and more frequent basis, the data base for mixing height determination will help reduce the uncertainty that now exists.

A related issue is the vertical resolution contained in PAQSMs. Most models for ozone extend no more than about 3 km above ground level and contain one to six vertical layers that may or may not be spatially and temporally variable. Is the gradient transport (K-theory) approximation that is often used to describe turbulent transport between the layers adequate? Are the vertical velocities generated by the highly processed wind field realistic? In most cases of regular terrain and well-behaved flow the vertical exchange between layers in the current models appears to be credible. In complex terrain and complex flow situations with possible internal boundary layers, however, the representation of vertical exchange processes may not be adequate. In an application of the Urban Airshed Model to the Tokyo metropolitan area,[5] Wakamatsu notices that the magnitude of mixing appears too great between the three vertical layers comprising the well-mixed region. Model results showed little vertical gradient between these layers while extensive aircraft measurements over the area during the simulation period showed distinct areas of ozone maxima just below the mixing height. Better representations of vertical transport and diffusion may be needed in the models, especially for complex flow situations.

I would now like to turn to the area of data requirements for PAQSMs, and restrict my comments to emission inventories. Historically emission inventories have been developed by groups of people often distinct from those groups performing the air quality modeling. This has often caused communication gaps between the groups and misunderstandings of the capabilities of the inventory specialists and the needs of the modelers. The modeler may have great anxiety about using a wind measurement, for example, that is given to him with a specified uncertainty of 30 percent, while having no qualms about using emissions inventory data that usually come with no uncertainty estimates. This double standard between emissions input data and other categories of model input data is unfortunate because it is the emissions, after all, that we have chosen as the independent variable on which to perform perturbations (control strategies) for modulating the response of the dependent

variable, ozone concentrations. In fact, modelers often use the results of their simulations in a gross sense to perform quality assurance of the emissions inventory. Glaring defects in the inventory often show up as anomalies in the predicted concentration fields. The inventory specialists can then be alerted, and another iteration of inventory estimates may follow. Less obvious problems in the inventory are more difficult to detect in this way.

In the Critical Review, Dr. Seinfeld states "Emission inventories will always possess, no matter how good our efforts are, varying levels of uncertainty in their different components." Looking at the multistep process of emission inventory estimation one can readily see that this is certainly a valid statement. Our job, as modelers and users of PAQSM-predicted data, is to understand some of the basic uncertainties in the emissions data base and try to factor that knowledge in our use of the models. There is, as yet, no reliable method of objectively estimating the uncertainty in the emissions data. Quantifying the uncertainties is left to the judgment of the emissions inventory specialists. There has been an attempt recently to do just that. The "Delphi" technique was used where a panel of inventory experts subjectively provided their estimates of uncertainty for various aspects of the emissions inventory process for the 1980 U.S. NAPAP inventory.[6] Table I shows the consensus of the panel for selected steps in the emissions inventory construction process for VOC, NO_x, and CO emissions. In the table the percent error, p, of a variable Y, is defined such that 90 percent of the values lie within the range $(1 - p/100)E$ and $(1 + p/100)E$, where E is the mean value of Y. Generally the VOC uncertainties are greater than those for NO_x or CO and the temporal and species allocation steps contribute significantly to the overall error. Stack test and material balance processes refer to point source emissions, while the remainder of the list refers to area source emissions.

Table II indicates the composite error for the final hourly gridded emissions inventory that the modelers would use. Biogenic VOC emissions have been added to the list for comparison. Obviously the VOCs contain the greatest amounts of uncertainty overall, although the estimated errors in the other species are not small. In addition to these errors we know that there are systematic underestimates of the VOCs because of certain categories of area sources that traditionally have not been considered. Dr. Seinfeld gave some indication of this in mentioning the discrepancies one finds when comparing the VOC/NO_x ratio in the emissions inventory with that from 6:00–9:00 A.M. ambient data. With each new generation of emissions inventory, the methods are improved and the overall errors are reduced somewhat. For example, in the development of the more recent 1985 U.S. NAPAP inventory, significant improvements have been made in the specification of area source methodologies. These include the compilation of more detailed activity data, reevaluation of spatial allocation surrogate indicators, and development of methodologies for source types that previously were not included in the inventories.

Table I. Uncertainty estimates from the 1980 NAPAP anthropogenic emissions inventory.

Source of uncertainty	Percent error		
	VOC	NO_x	CO
Stack test	25	25	25
Material balance	50	25	25
Mobile	50	30	30
Seasonal allocation	10	10	10
Daily allocation	25	25	25
Hourly allocation	75	50	75
Species allocation	100	25	—
Spatial allocation	25	25	25

Table II. Composite uncertainty estimates from all sources of error for 1980 ROM grid-level hourly emissions input data.

	Percent error	
	Point and area sources	Area sources only
Speciated VOC (anthropogenic)	64	74
Speciated VOC (biogenic)	—	109
Speciated NO_x	32	33
CO	49	54

The basic modeling question related to emissions is how does the significant uncertainty in the inventory relate to how the models are being used. How do we interpret the results from a control strategy PAQSM simulation where we have reduced VOC emissions by 50 percent when the estimated error in the hourly gridded inventory is greater than 60 percent? One must be even more careful with interpreting NO_x control strategy results where the resulting ozone concentrations can either increase or decrease depending upon the absolute VOC and NO_x levels and the ratio between them. Because of the nonlinearity of the photochemical smog system, if we have significant errors in the amounts of precursors in the system we may not even have the direction of ozone change correct under conditions of NO_x control. Clearly more effort must go into reducing the remaining uncertainties in the emission inventories, to the maximum practical extent, to make them more useful in air quality planning and analysis.

Regional Scale PAQSMs

In the Critical Review Dr. Seinfeld discussed ozone air quality models on spatial scales up through the urban scale (~200 km). In recent years there has been significant progress as well in developing and applying models on a regional scale (~1000 km) for estimating region-wide ozone concentration patterns.[7] The need for these models arose from the realization that high ozone concentration episodes, especially in the Eastern U.S., were often characterized by interurban transport of ozone and precursor species on scales of hundreds of kilometers and several days of transport time. A number of three-dimensional grid models have been developed to simulate air quality on regional scales, including two that were specifically developed for the regional ozone problem. They are EPA's Regional Oxidant Model (ROM)[8] and the Regional Transport Model (RTM-III)[9] developed by Systems Applications, Inc. Other regional models include the oxidant species as part of the acid deposition process which they focus on. At present the ROM is being applied to the Northeast and Southeast U.S., and the RTM-III's applications include the Eastern and Midwestern U.S., California's Central Valley, and Western Europe. Spatial resolution in regional models is usually coarser than that in urban models because of coarser resolution in the available input data and also to reduce the higher computational expense associated with the larger model domain. While the grid cell size in urban models is usually from 2–10 km, the cell size in regional models runs from 20–80 km.

The chemical and physical processes responsible for photochemical smog on the urban scale discussed in the Review are also important on the regional scale. Several other processes are significant on the regional scale that may be effectively ignored on the urban scale. These processes have time and space scales of significance that are greater than the urban models can treat. For instance, summertime cumulus clouds can efficiently transfer considerable amounts of mass vertically from the lower boundary layer into the cloud layer

with little intervening entrainment. The material at the higher altitude is then subject to transport by higher speed winds, especially the material remaining at night when the upper boundary layer is decoupled from the surface inversion layer. Entrainment of this material into the boundary layer far downwind can, in turn, affect the photochemical cycle the next day.

Biogenic emissions, especially of VOCs, are potentially significant on regional scales. These include, principally, emissions of isoprene and monoterpenes, from various species of trees, crops, and grasses. It is estimated that for the Northeast U.S. the total mass of VOCs emitted from biogenic sources is on the same order of magnitude as that from anthropogenic sources. The great difference between the source types is in the spatial distribution of the emissions. Anthropogenic emissions are concentrated in major urban centers and industrial complexes. By contrast, biogenic emissions are spread over very large stretches of mostly agricultural, rural, and remote areas with emission flux values considerably smaller than anthropogenic values from significant sources. Because the anthropogenic emissions far outweigh the biogenics in the vicinity of most major urban areas, urban scale models can effectively neglect the biogenic emissions. However, on the regional scale where biogenic VOCs can alter the reactivity of the background environment, the effect must be considered. Recent modeling studies with the ROM have shown that when emissions from large NO_x sources are introduced into relatively rural or remote areas of the domain, the presence of biogenic VOCs can appreciably enhance the photochemical production of ozone.

The specification of a three-dimensional wind field is another problem on the regional scale. The Critical Review discussed some of the uncertainties of wind field analysis on the urban scale. The location of trajectories in the Los Angeles basin was examined using a complete wind observation network that was available for the analysis as well as under conditions in which the network was selectively degraded. Some of the calculated trajectories were significantly different under the conditions of the degraded network.[10] On the regional scale there is even less determinism in the wind observation network. While the Los Angeles study cited above used 10 upper air radiosonde stations with observations available every 4 hours from a special field study data base, the typical separation distance of radiosonde stations in the North American air monitoring network is 300–500 km with twice daily observations. The surface wind network is considerably more dense, but these measurements are not as spatially representative of large scale flows as the upper air observations. Therefore the upper air measurements are weighted more heavily in constructing wind fields for use in PAQSMs.

If different interpolative techniques are applied to the wind data base, gridded wind fields will be represented differently over time and space. Admittedly the various wind fields will appear quite similar for a given time, but if trajectories are followed for each wind field from the same starting location over the time and space scales characteristic of regional modeling, the trajectory endpoints may occur at widely separated locations.[11] Obviously this has serious implications for correctly representing spatial patterns of pollutant concentrations on the regional scale and for evaluating emissions control strategies with the PAQSMs.

Because of this lack of determinism in regional wind field analyses, it has been suggested that simulation results from regional scale PAQSMs be used in a probabilistic or quasi-deterministic mode, as opposed to a strictly deterministic mode. In the deterministic mode, the model prediction for a given time and location is used by the air quality analyst in a strict sense (i.e., without consideration of expected variance from any source of error). This has been the usual mode of operation in interpreting simulation model results. In the probabilistic mode a given receptor location would be characterized by an expected probability distribution of concentrations for a given time, based on some finite number of possible wind field realizations. (The probability concept could be extended to variables other than the wind in model simulation, but we choose to focus on the transport variable in this analysis.) Since the probabilistic mode is quite difficult to implement at present we are using a quasi-deterministic mode with our ROM model results. Here we analyze the model results in an aggregated sense. That is, if we want to focus on a particular time period we aggregate model results for that time period from groups of receptor locations having certain common characteristics, such as all urban receptors or rural downwind receptors. If we focus on particular receptors or locations, then we aggregate or average model results over longer time periods. For example, we might analyze the maximum predicted ozone concentration for each receptor location over an entire episode or over a week or longer simulation period.

C. Shepherd Burton, left, and Kenneth L. Schere

The lack of determinism in wind field analysis may not be as important a factor in urban scale modeling because of the shorter time and space scales, although if model results from urban PAQSMs are strictly interpreted in terms of time and location, then the determinism question does come into play as evidenced by Kessler's trajectory analyses.[10] Wind fields generated by prognostic meteorological models, as discussed by Dr. Seinfeld, may perhaps mitigate the determinism problem in wind field generation, especially where four dimensional data assimilation techniques are used in conjunction with the model, although there will always be a stochastic component to atmospheric flows that will be difficult to capture in a deterministic analysis. The probabilistic mode of interpreting simulation model results is therefore still appropriate when the PAQSM is driven by prognostically-generated winds.

Regional PAQSMs are currently being used to provide an assessment of wide area impacts of mostly urban-oriented precusor emission controls. This includes analyses of the impacts for rural, agricultural, and forested areas for episodic and seasonal exposures. The interurban transport of ozone and precursor species is also being studied with regional models. In addition, regional simulation results will be used to provide initial and boundary conditions to urban models for specific episode simulations in an integrated modeling assessment for individual Northeast Corridor cities (ROMNET).[12]

Model Evaluation

In the Critical Review Dr. Seinfeld gave sufficient attention to model evaluation and sensitivity analysis with regards to PAQSMs. I would like to focus on a few of the points that I feel are most significant on this topic. First, the difference between a valid model and a verified or evaluated mod-

el is important. A valid model, in this context, is one in which the requisite physical and chemical processes have been adequately included and correctly represented in the simulation process. For example, the chemical representation of photochemical smog processes have been simulated with an up-to-date kinetic mechanism that has been separately evaluated with smog chamber experimental data. The transport mechanism should have been tested against analytic flow representations with exact solutions as well as perhaps tracer experiments in the atmosphere. A verified model is one in which the entire simulation "package" or model has successfully been tested against ambient observational data, such as maximum ozone concentrations. It is possible for a valid model to perform poorly in atmospheric simulations, just as it is possible for a non-valid, or highly empirical model to perform well. The key diagnostic process involved in evaluation is to examine whether a valid model is performing well for the right reasons, and for cases where poor performance is shown, to try to understand the cause of the errors.

Diagnosing model errors in a valid model can be particularly difficult. There are a number of reasons for this and Dr. Seinfeld has mentioned a few of them. First, there is no measured quantity equivalent to a volume-integrated grid model concentration prediction; therefore no absolute measure of model performance exists. Point measurements are invariably used for comparison with model predictions, and questions about the "representativeness" of point measurements are always an issue, particularly as the model's spatial resolution decreases and grid cell size increases. Another problem in model diagnostics is the inherent difficulties in reconstructing the meteorological and emissions fields on the day in question. As evidenced by the discussions above on the uncertainties in the emissions data base and the lack of determinism in the wind fields, the uncertainties associated with the model input data on any one day used for simulation may be very large. One must therefore very carefully weigh the potential influence of these input data problems on model results before ascribing model bias to errors in the model formulation and process simulation. Sensitivity analysis will help to separate the effect of input data uncertainties. However, a variable to which the model is quite sensitive and which carries significant uncertainty will continue to be a problem in the model evaluation process.

When developing a protocol for evaluation of a particular model one should keep in mind the intended use of the model. In most cases PAQSMs are used for assessment of the degree of precursor control required to bring the maximum ozone concentrations to the level of the national standard (0.12 ppm). Therefore what the air quality policy analyst is really interested in is not necessarily the model's ability to predict the maximum ozone concentration, but rather to predict $d(O_3)/dS$, where S is the source emissions term. Correct estimation of the absolute ozone concentrations may be a necessary condition for this, but it is not sufficient. Unfortunately, existing data bases, particularly for source emissions, are inadequate for assessing $d(O_3)/dS$ from ambient or model-simulated data bases. As higher quality emission inventories with less inherent uncertainty become available, we may be able to start this type of assessment. Also, the use of consistent procedures in developing inventories will make the comparisons over time more meaningful. However, a parallel improvement will be needed in air quality monitoring as well as emission inventory development. To help assess whether our baseline inventories are accurate and whether we are getting the expected reductions in emissions over time that our existing control programs say we are, we need more and better quality monitoring of NO_x and VOCs nationwide. There has been some improvement in recent years in monitoring for these species, but it tends to be in special field programs that do not give the needed time record of data to track trends. To assess PAQSMs in the sense in which they are typically used we will need improved ambient air quality data bases.

Future Directions

The Critical Review discusses three areas where research is needed in the near future: wind field generation, model performance evaluation, and sub-grid scale processes. These are certainly critical components in the PAQSM system and sustained long-term research programs in these areas are needed to continue to produce future generations of more credible models. Other research areas I would include are vertical exchange processes and atmospheric chemistry. Dr. Seinfeld states his opinion that contemporary PAQSMs have reached a level of accuracy that may be difficult to improve upon in the near future. Focusing on ozone alone and weighing the deficiencies in the existing data bases, this statement may be true. However if we look at the predictions of the PAQSMs for other key components of photochemical smog, such as PAN, OH, or VOCs, there can be considerable differences from model to model in the predictions of these species concentrations, indicating that while we may be doing adequately at ozone prediction we are not certain yet that it is for all the right reasons.

Given the fairly sophisticated level of science incorporated into most contemporary PAQSMs, it appears we now have well outpaced the level of sophistication in the data bases available to us for use with the models. Resources must be allocated to improve these data bases and thought must be given to the proper way to incorporate inherently uncertain data into inherently deterministic models. New ways of thinking about model evaluation are needed as are new ways of interpreting model results. The relationship between probabilistic PAQSM results and the present form of the NAAQS should be established.

Finally, the interaction of urban and regional ozone with other scales should be considered for future work. Contributions of ozone from the free troposphere and the stratosphere may, at times, contribute significantly to boundary layer ozone. This is especially true if we look at longer time averages or seasonal exposure of crops and forests. If the U.S. moves toward a secondary ozone air quality standard in addition to the existing primary standard, welfare effects will become a major concern. With the lower concentrations associated with longer time averages the models will have to more adequately distinguish between background ozone and local production when the latter may be of the same magnitude as the former. In this situation we will need a better way to characterize the background ozone burden than that which we presently use in PAQSMs. Possibilities include a coupling or feedback mechanism between models of the free troposphere or stratosphere with our regional PAQSMs. In western Europe where the welfare effects of ozone pollution have been of concern for some time there have been attempts to use a two-dimensional model of the free troposphere to provide boundary conditions for a three-dimensional regional PAQSM.[13] Also, as concerns of global climate change increase and the two-way interaction of local and regional pollution on global climate become of interest we will need techniques of coupling the disparate spatial and temporal scales of local, regional, and global models.

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I appreciate the privilege and opportunity to comment on Professor John Seinfeld's review of "Ozone Air Quality Models." Professor Seinfeld is among the originators of the Eulerian (grid) modeling approach for simulating ozone formation in urban environments. In its scope, depth, and currency, his review reflects what one would expect from a leading contributor to the field of photochemical ozone modeling.

I will not offer criticisms of Seinfeld's excellent review. As might be expected, on many matters dealing with the calculation of peak ozone concentrations we share similar views. However, while I may not disagree with Professor Seinfeld, he may disagree with some of my comments here.

My discussion represents an extension of Seinfeld's review—a discussion that focuses on what I believe is his principal conclusion, one that is consistent with our ozone modeling experience at Systems Applications, Inc. That conclusion is this: We (the technical community) can, using the Urban Airshed Model (UAM), reliably reproduce point observations of peak 1-hour average ground-level ozone concentrations in urban environments. We can also, with equal reliability, reproduce spatial patterns of 1-hour ozone concentrations over periods of one to several days and over regions as small as a few thousand square miles to as large as 20,000 mi^2, an area about one-half the size of Ohio. Further, our ability to reproduce peak concentrations is better than 30 percent of the observation when the calculated and observed concentrations pairs are matched in space and time; when we relax the stringent, space-time matching requirement, we seem to be able to reproduce peak, point observations within approximately 15 percent of the observed maximum. Such performance equals or exceeds that of any other EPA-guideline model.

I am not suggesting that we know everything we need to know or could know, and, therefore, that more research in photochemical modeling and related areas is not necessary. Indeed, later in this discussion I will provide specific suggestions, which are consistent with those recommended by Seinfeld, where additional work is needed.

I am suggesting, on the basis of the evidence in Seinfeld's review and in my discussion here, that grid models in general—and the Urban Airshed Model in particular—should no longer be viewed only as arcane research tools of limited applicability and only useful in a state in which above average resources are allocated to address air quality issues, or those with perceived "infinite" resources, patience, and propensity to be technically unique, or those with a compelling need to challenge regulatory arbitrariness. Instead, it is my position that grid models should be viewed as tools—regulatory tools—that offer air quality planners and managers a sound approach for identifying practical, comprehensive, cost-effective, and, when necessary, innovative ozone attainment strategies. Thus, instead of arguing about whether they should be used, the debate should shift to when and how they can best be used as part of air quality management practices in the United States and to how their cost performance can be improved.

One would be correct to infer from my discussion that I believe the use of EKMA—the current EPA-accepted regulatory alternative to the Urban Airshed Model—should be discouraged, except in limited situations. Indeed, it is my position that the regulatory roles of EKMA and the UAM in developing ozone attainment strategies and demonstrating attainment should be reversed—UAM should be the workhorse and EKMA should be used in special (simple) situations. I will mention some of those simple applications shortly.

In the Congress, at the EPA and in several states, discussions are underway that involve, among other topics, how best to proceed toward the attainment of the federal ozone standard. A central issue in those discussions is which emis-

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